

Quantum tunneling between paramagnetic and superconducting states of a nanometer-scale superconducting grain placed in a magnetic field.

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(February 1, 2008)

We consider the process of quantum tunneling between the superconducting and paramagnetic states of a nanometer-scale superconducting grain placed in a magnetic field. The grain is supposed to be coupled via tunneling junction to a normal metallic contact that plays a role of the spin reservoir. Using the instanton method we find the probability of the quantum tunneling process and express it in terms of the applied magnetic field, order parameter of the superconducting grain and conductance of the tunneling junction between the grain and metallic contact.

Recent advances in manufacturing of small electronic devices posed several questions in the theory of nanometer-size superconductors related to their prospective applications [1]. One of the key issues is the behavior of ultra-small superconductors, of the dimensions much less than the coherence length ξ in the presence of a magnetic field. Of a special interest from both fundamental and practical point of view are the dynamical processes of switching between the superconducting and paramagnetic states. Small grains can experience spontaneous transitions due to quantum fluctuations. In this Letter we investigate the process of quantum tunneling between the superconducting and paramagnetic states of an ultra-small superconductor.

In geometrically restricted superconductors the Zeeman effect suppresses superconductivity at magnetic fields exceeding $H_{spin} = \Delta/\sqrt{2}\mu_B$ where Δ is the order parameter [2–4]. The orbital effect in small superconductors, which usually plays a major role, was discussed in a pioneering work by Larkin [5]: In a dirty spherical grain, $\Delta\tau \ll 1$, τ is the normal excitation relaxation time, the orbital effect leads to suppression of superconductivity at $H_{orb} \sim \Phi_0/(r\sqrt{D/\Delta})$, where $\Phi_0 = hc/2e$, D is the diffusion coefficient, and r is the radius of the grain.

Tunneling switching effects appear in the paramagnetic limit $H_{spin}/H_{orb} \sim \sqrt{\Delta/d}\sqrt{l/r} \ll 1$, where $l = v_F\tau$ is the mean free path, and d is the mean energy level spacing. In the ballistic case ($l \simeq r$) this limit is achieved only if $\Delta < d$ corresponding to the strongly fluctuating regime [6]. However in a platelet geometry with magnetic field applied along the film $H_{spin}/H_{orb} \sim \sqrt{\Delta/d}\sqrt{lb/S}$, where b is the thickness and S is the area of the sample; thus the paramagnetic limit can be easily achieved along with condition $\Delta \gg d$ even in the ballistic case if the ratio b/\sqrt{S} is sufficiently small.

We focus on the case where the Zeeman effect dominates the orbital one while the order parameter Δ is larger than the mean level spacing d and investigate the process of quantum tunneling between superconducting and paramagnetic states. Since these two states are characterized by different values of the total spin, such quan-

tum tunneling process can occur only in presence of processes allowing for non-conservation of the total spin. We consider the grain weakly coupled with a normal metallic lead (plate) that plays a role of a spin bath. Our final result for the probability of the quantum tunneling between the superconducting and paramagnetic states is

$$P \sim \exp [N \ln(\beta\delta EG/\Delta_0)] \quad (1)$$

where the numerical coefficient $\beta \approx 1.1$, the factor N is the number of polarized electrons in the paramagnetic state of the grain, G is the conductance of the tunneling junction between the grain and the metallic lead measured in units e^2/h , Δ_0 is the order parameter of the grain in the superconducting state and $N\delta E$ is the total energy difference between the grain's superconducting and paramagnetic states. The factor N is related to the applied magnetic field H and the average density of states ν as $N = 2\nu\mu_B H$ with $\mu_B = |e|\hbar/2mc$. The energy difference per one state δE is related to the magnetic field deviation δH from the magnitude at which the thermodynamic phase transition occurs via $\delta E = \mu_B\delta H$. The result (1) is valid as long as $\delta E/\Delta \ll 1$, the general case $\Delta \sim \delta E$ is more complicated and we leave it for future study. The meaning of our answer (1) can be understood as follows. The probability of a single tunneling process is $(\delta E/\Delta_0)G$, then the probability of having N of them simultaneously in order to transit to paramagnetic state is simply $[(\delta E/\Delta_0)G]^N$.

The model. We consider a system of a superconducting grain and a metallic plate coupled via weak tunneling

$$\hat{H} = \hat{H}_g + \hat{H}_M + \sum_{k,k'} t_{kk'} [\hat{\psi}_{k\sigma}^\dagger \hat{d}_{k'\sigma} + \hat{d}_{k'\sigma}^\dagger \hat{\psi}_{k\sigma}]. \quad (2)$$

where \hat{H}_g and \hat{H}_M are the Hamiltonians of the grain and metallic plate, $\hat{\psi}^\dagger(\hat{\psi})$ and $\hat{d}^\dagger(\hat{d})$ are the creation (annihilation) operators of electrons of the grain and of the metal respectively and $t_{kk'}$ is the electron tunneling matrix element between the grain and metal. Electrons of metallic plate are described by the free-fermion Hamiltonian

$$\hat{H}_M = \sum_{k'} \hat{d}_{k'\sigma}^\dagger \zeta_{\sigma k'} \hat{d}_{k'\sigma}.$$

while the grain is described by the BCS model

$$H_g = \sum_k \psi_k^\dagger [\xi_k - h\sigma_z] \psi_k - \lambda \sum_{k1,k2} \psi_{k1\uparrow}^\dagger \psi_{k1\downarrow}^\dagger \psi_{k2\downarrow} \psi_{k2\uparrow}, \quad (3)$$

where ξ_k are the exact eigenvalues (measured with respect to the chemical potential) of the noninteracting Hamiltonian, λ is the coupling constant, and the magnetic field h , pointing along the z -axis, is measured in the energy units $h = \mu_B H$.

Quantum tunneling. The amplitude of the tunneling process between the initial and final states is

$$A = \langle f | T_t e^{-i \int_{t_i}^{t_f} \hat{H}(t) dt} | i \rangle, \quad (4)$$

where the Hamiltonian $\hat{H}(t)$ is written in the interaction representation: the noninteracting part includes the metal Hamiltonian H_M and the first (free-fermion) term of grain Hamiltonian (3) while the interaction part includes the BCS interaction and electron tunneling between the grain and metal. We will consider a process of quantum tunneling from pure superconducting state (initial state) to the paramagnetic state with order parameter $\Delta = 0$. The electron tunneling between the grain and metal will be treated as a perturbation assuming that the tunneling matrix elements $t_{kk'}$ are small. The paramagnetic state has a nonzero total spin S which is formed by the polarized electrons with $|\xi_k| < \tilde{\xi}$ such that $S = \nu \tilde{\xi}$. During the quantum tunneling process the spin of the grain increases from zero to S , thus there must be $2S$ electron tunneling processes between the grain and metal and first nonzero contribution in expansion of Eq.(4) in tunneling element emerges only in $N = 2S$ order. It is clear that the paired states which are destroyed by the electron tunneling are those with $|\xi| < \tilde{\xi}$. Expanding Eq.(4) in t we have

$$A = \langle f | \prod_{|\xi_k| < \tilde{\xi}} \int dt_k T_t e^{-i \int_{t_i}^{t_f} \hat{H}(t) dt} \sum_{k'} t_{kk'} \times [\hat{\psi}_{k\sigma}^\dagger(t_k) \hat{d}_{k'\sigma}^\dagger(t_k) + \hat{d}_{k'\sigma}^\dagger(t_k) \hat{\psi}_{k\sigma}(t_k)] | i \rangle. \quad (5)$$

In the absence of coupling between the grain and metal the initial and final states of the system are the products of the corresponding initial and final states of the grain and metal $|i\rangle = |i_G\rangle |i_M\rangle$, $|f\rangle = |f_G\rangle |f_M\rangle$, thus in the leading order in tunneling matrix element the quantum mechanical average of operators \hat{d} in (5) can be directly implemented. Since the total spin of the metallic plate decreases during the quantum tunneling process the only relevant matrix elements are those that correspond to creation of electrons with spin down and annihilation of electrons with spin up

$$\begin{aligned} \langle f_M | d_{k\downarrow}^\dagger(t) | i_M \rangle &= e^{i\zeta_{k\downarrow} t}, & \zeta_{k\downarrow} > 0 \\ \langle f_M | d_{k\uparrow}(t) | i_M \rangle &= e^{i|\zeta_{k\uparrow}| t}, & \zeta_{k\uparrow} < 0. \end{aligned}$$

The initial state of the metal is the Fermi sea while its final state having N electron-hole excitations is characterized by the set of excitation energies $\zeta_{k'\alpha}^{\{p\}}$ where the index k' labels the quantum number of the excitation p . Now assuming that tunneling matrix elements are independent $t_{k,k'} = t$ the amplitude can be written as

$$A = t^N < f_G | T_t \prod_{|\xi_k| < \tilde{\xi}} \int dt_k e^{-i \int_{t_i}^{t_f} \hat{H}(t) dt} \sum_{\text{Per } p(k)} e^{i\zeta_{k'}^{\{p(k)\}} t_k} \times [\hat{\psi}_{k\uparrow}^\dagger(t_k) \theta(-\zeta_{k'}^{\{p(k)\}}) + \hat{\psi}_{k\downarrow}(t_k) \theta(\zeta_{k'}^{\{p(k)\}})] | i_G \rangle \quad (6)$$

where the sum goes over all excitation permutations $p(k)$. Since we consider only the case $\delta E \ll \Delta$ we can simplify the problem assuming that the energy of a typical excitation in the metal is much less than Δ . In this case we can neglect the energies $\zeta_{k'}^{\{p\}}$ in (6) and using the Heisenberg representation we write the amplitude (6) as

$$A = N! t^N < f_G | \prod_{|\xi_k| < \tilde{\xi}} \int dt_k [\hat{\psi}_{k\uparrow}^\dagger(t_k) \theta(-\zeta_{k'}^{\{p(k)\}}) + \hat{\psi}_{k\downarrow}(t_k) \theta(\zeta_{k'}^{\{p(k)\}})] | i_G \rangle, \quad (7)$$

where a specific permutation $p(k)$ was chosen.

The probability P of the tunneling process is obtained by integrating of $A^* A$ over all possible quantum states of the metal

$$P \sim \frac{\nu_M^N}{N!} \int d\zeta^{\{1\}} \dots d\zeta^{\{N\}} A^* A \delta(N \delta E - \sum_p |\zeta^{\{p\}}|), \quad (8)$$

where ν_M is the density of states of the metal.

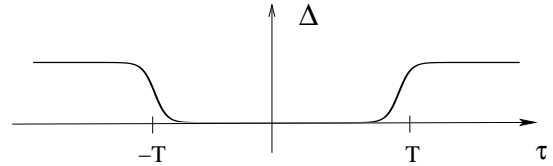


FIG. 1. Dependence of the order parameter Δ on time τ . The region $\tau > 0$ is the mirror reflection of the “physical” region $\tau < 0$. The superconducting state corresponds to the regions $|\tau| > T$ while the paramagnetic one to $|\tau| < T$.

To find the value of A we shall use the instanton method turning to use the Euclidean time $t \rightarrow -i\tau$. Taking initial and final times as $\tau_i = -\infty$, $\tau_f = 0$ we present the amplitude A as

$$A = N! t^N < f_G | S(0, -\infty) | i_G \rangle$$

with the evolution operator

$$S(\tau_2, \tau_1) = \prod_{|\xi_k| < \tilde{\xi}} \int_{\tau_1}^{\tau_2} d\tau_k [\hat{\psi}_{k\uparrow}^\dagger(\tau_k) \theta(-\zeta_{k'}^{\{p(k)\}}) + \hat{\psi}_{k\downarrow}(\tau_k) \theta(\zeta_{k'}^{\{p(k)\}})]. \quad (9)$$

In principle, the instanton method should be applied to the amplitude A directly, but it is more convenient to consider the product A^*A presenting A^* as $A^* = N! t^N < i_G | S^\dagger(\infty, 0) | f_G >$ and writing the product A^*A as

$$A^*A = < i_G | S^\dagger(\infty, 0) | f_G > < f_G | S(0, -\infty) | i_G > \\ = < i_G | S^\dagger(\infty, 0) S(0, -\infty) | i_G >,$$

where it was used that by construction the Euclidean evolution operator S brings the grain from initial $|i_G >$ to the final $|f_G >$ state: $S|i_G > = |f_G >$. Now the instanton process has the following structure (see Fig.1): the evolution begins at $\tau = -\infty$ from the superconducting state, then at $\tau \approx -T$ the system turns into the paramagnetic state and stays there till it turns back to the superconducting state at $\tau \approx T$. The artificial part of the process ($\tau > 0$) is the mirror reflection of the “physical” process with $\tau < 0$. The advantage of this representation is that now the new initial ($\tau = -\infty$) and final ($\tau = \infty$) states are identical and therefore we can use the convenient functional representation for A^*A

$$A^*A = [N! t^N]^2 \int D\psi^\dagger D\psi e^{\int \mathcal{L} dt} \prod_k \int d\tau_{1k} d\tau_{2k} \\ \times \left[\psi_{k\uparrow}(\tau_{1k}) \psi_{k\uparrow}^\dagger(\tau_{2k}) \theta(-\zeta_{k'}^{\{p(k)\}}) \right. \\ \left. + \psi_{k\downarrow}^\dagger(\tau_{1k}) \psi_{k\downarrow}(\tau_{2k}) \theta(\zeta_{k'}^{\{p(k)\}}) \right], \quad (10)$$

with the Lagrangian

$$\mathcal{L} = -\frac{1}{\lambda} \Delta^* \Delta - \sum_k \psi_k^\dagger [\partial_\tau + \xi_k - h \sigma_z] \psi_k \\ - \Delta \psi_{k\uparrow}^\dagger \psi_{k\downarrow}^\dagger - \Delta^* \psi_{k\downarrow} \psi_{k\uparrow}. \quad (11)$$

The integration over the fermionic fields in (10) should be implemented exactly while the assumed integration over $\Delta(\tau)$ will be done with the saddle point accuracy. Now taking integrals in (8) for the probability we obtain

$$P = e^{N \ln(N \delta E t^2 \nu_M)} \int D\psi^\dagger D\psi \prod_k \int d\tau_{1k} d\tau_{2k} \\ \times e^{\int \mathcal{L} d\tau} [\psi_{k\uparrow}(\tau_{1k}) \psi_{k\uparrow}^\dagger(\tau_{2k}) + \psi_{k\downarrow}^\dagger(\tau_{1k}) \psi_{k\downarrow}(\tau_{2k})],$$

and finally integrating over the fermionic fields we obtain

$$\ln P = N \ln(N \delta E t^2 \nu_M) + \sum_k \text{Tr} \ln[\partial_\tau + \mathcal{H}_k] \\ - \frac{1}{g} \int d\tau \Delta^*(\tau) \Delta(\tau) + \sum_k \ln Z_k, \quad (12)$$

where $Z_k = \text{Tr} \int d\tau_1 d\tau_2 \hat{G}_{1k}(\tau_1, \tau_2)$,

$$\mathcal{H}_k(\tau) = \begin{bmatrix} \xi_k - h & \Delta(\tau) \\ \Delta^*(\tau) & -\xi_k - h \end{bmatrix}, \quad (13)$$

and the matrix Green function

$$\hat{G}_{1k}(\tau_1, \tau_2) = \begin{bmatrix} G_{1k}(\tau_1, \tau_2) & F_{1k}(\tau_1, \tau_2) \\ F_{1k}^\dagger(\tau_1, \tau_2) & \bar{G}_{1k}(\tau_1, \tau_2) \end{bmatrix}. \quad (14)$$

is defined by the equation

$$[\partial_{\tau_1} + \mathcal{H}_k(\tau_1)] \hat{G}_{1k}(\tau_1, \tau_2) = \delta(\tau_1 - \tau_2). \quad (15)$$

Instanton equations. To find the instanton equations we take the functional derivative of Eq.(12) with respect to Δ^* obtaining

$$\frac{1}{\lambda} \Delta(\tau) = \sum_k f_{1k}(\tau) + f_{2k}(\tau), \quad (16)$$

where the Green function $f_1(\tau) = F_1(\tau, \tau)$ emerges from the variation derivative of $\text{Tr} \ln[\partial_\tau + \mathcal{H}_k]$ in (12) and f_2 emerges from the functional derivative of the Green function \bar{G}_1

$$f_2(\tau) = Z_k^{-1} \frac{\delta}{\delta \Delta^*(\tau)} \int d\tau_1 d\tau_2 \text{Tr} G_{1k}(\tau_1, \tau_2). \quad (17)$$

Combining Eq.(15) with the same equation written in the transposed form one can find the equation that defines the function f_1 in terms of only diagonal Green functions

$$\partial_\tau \hat{g}_{1k}(\tau) + [\mathcal{H}_{0k}(\tau), \hat{g}_{1k}(\tau)] = 0, \quad (18)$$

where

$$\hat{g}_{1k}(\tau) = \begin{bmatrix} g_{1k}(\tau) & f_{1k}(\tau) \\ f_{1k}^\dagger(\tau) & \bar{g}_{1k}(\tau) \end{bmatrix} = \hat{G}_{1k}(\tau, \tau), \quad (19)$$

and \mathcal{H}_0 is given by Eq.(13) with $h = 0$. Writing Eq.(18) in components we get

$$\begin{aligned} \partial_\tau \tilde{g}_{1k} + \Delta f_{1k}^\dagger - \Delta^* f_{1k} &= 0, \\ \partial_\tau f_{1k} + 2\xi_k f_{1k} - 2\Delta \tilde{g}_{1k} &= 0, \\ -\partial_\tau f_{1k}^\dagger + 2\xi_k f_{1k}^\dagger - 2\Delta^* \tilde{g}_{1k} &= 0, \end{aligned} \quad (20)$$

$$\partial_\tau s_{z1k} = 0, \quad (21)$$

where the variables $\tilde{g}_1 = [g_{1k} - \bar{g}_{1k}]/2$, $s_{z1k} = -[g_{1k} + \bar{g}_{1k}]/2$ were introduced instead of components g_1 and \bar{g}_1 . Eqs.(20) are very similar to the well known Eilenberger [7] equations and possess the same invariant $\tilde{g}_{1k}^2 + f_{1k}^\dagger f_{1k} = \text{const}$. Now we turn to the function $f_2(\tau)$: Using the definition of the Green function (15) one can take the variational derivative in Eq.(17) obtaining

$$f_{2k}(\tau) = -Z_k^{-1} [f_k^{II}(\tau) g_k^I(\tau) + \bar{g}_k^{II}(\tau) f_k^I(\tau)] \quad (22)$$

where g_k^I, f_k^I are the components of the matrix Green function

$$\hat{g}_k^I(\tau) \equiv \begin{bmatrix} g_k^I(\tau) & f_k^I(\tau) \\ f_k^{\dagger I}(\tau) & \bar{g}_k^I(\tau) \end{bmatrix} = \int d\tau_2 \hat{G}_{1k}(\tau, \tau_2) \quad (23)$$

and f_k^{II}, \bar{g}_k^{II} are the components of the matrix Green function $\hat{g}_k^{II}(\tau) = \int d\tau_1 \hat{G}_{1k}(\tau_1, \tau)$. Equations that determine

the functions \hat{g}^I and \hat{g}^{II} can be easily found by integrating Eq.(15) over τ_2 and transposed Eq.(15) over τ_1

$$\begin{aligned} \partial_\tau g_k^I(\tau) + \mathcal{H}_k(\tau) g_k^I(\tau) &= 1 \\ -\partial_\tau g_k^{II}(\tau) + g_k^{II}(\tau) \mathcal{H}_k(\tau) &= 1. \end{aligned} \quad (24)$$

Initial and final conditions. Initial and final conditions should be formulated for the Green function $\hat{g}_k^{\alpha,\beta}(\tau)$ which is defined with respect to the evolution operator $S^\dagger S$,

$$\hat{g}_k^{\alpha,\beta}(\tau) = \frac{\langle i_G | S^\dagger(\infty, 0) S(0, \tau) \hat{\psi}_k^\alpha \hat{\psi}_k^{\beta\dagger} S(\tau, -\infty) | i_G \rangle}{\langle i_G | S^\dagger(\infty, 0) S(0, -\infty) | i_G \rangle}$$

where a negative τ was chosen for concreteness. To find the function $\hat{g}_k(\tau)$ in the functional representation we add the source term $\int d\tau \mu_k^{\alpha\beta}(\tau) \tilde{\psi}_\alpha(\tau) \tilde{\psi}_\beta^\dagger(\tau)$ where $\tilde{\psi}$ is the Nambu spinor to the Lagrangian (11) and take the variation derivative of (12) with respect to $\mu_k^{\alpha\beta}(\tau)$ obtaining

$$\hat{g}_k(\tau) = \hat{g}_{1k}(\tau) + \hat{g}_{2k}(\tau),$$

where \hat{g}_{1k} is defined by Eq.(19) and the function

$$\hat{g}_{2k}(\tau) = \begin{bmatrix} g_{2k}(\tau) & f_{2k}(\tau) \\ f_{2k}^\dagger(\tau) & \bar{g}_{2k}(\tau) \end{bmatrix}$$

is related with g^I and g^{II} by

$$\hat{g}_{2k} = -\hat{g}_k^I \hat{g}_k^{II} / Z_k. \quad (25)$$

In the superconducting phase ($|\tau| \gg |T|$) the function \hat{g}_k should coincide with the equilibrium superconducting Green functions

$$\tilde{g}_k = \xi_k / 2 E_k, \quad f_k = \Delta / 2 E_k, \quad f_k^\dagger = f_k^*, \quad s_z = 0 \quad (26)$$

where $E_k = \sqrt{\xi_k^2 + \Delta^2}$, $\tilde{g}_k = [g_k - \bar{g}_k] / 2$, $s_{zk} = -[g_k + \bar{g}_k] / 2$. The function \tilde{g} is directly related with electron density on the level k by $n_k = 1 - 2\tilde{g}_k$ and the function s_{zk} is the z-component of the spin on the level k . Analogously, in the paramagnetic phase the Green function \hat{g} is

$$\tilde{g}_k = f_k = f_k^\dagger = 0, \quad s_{zk} = 1/2 \quad \text{for} \quad |\xi_k| < \tilde{\xi} \quad (27)$$

$$\tilde{g}_k = \text{sign} \xi_k / 2, \quad s_{zk} = f_k = f_k^\dagger = 0 \quad \text{for} \quad |\xi_k| > \tilde{\xi}. \quad (28)$$

In the absence of tunneling the physical Green function \hat{g} would coincide with \hat{g}_1 that obeys equations (20,21) conserving the quasiparticle spin. Therefore the function \hat{g}_1 in the paramagnetic state obeys the boundary condition (28) for any ξ while in the superconducting state it obeys the boundary conditions (26), so that $\hat{g}_2 \rightarrow 0$ in the superconducting phase.

Numerical solution. Solution of Eqs.(20) satisfying the necessary boundary conditions for a given configuration of the order parameter $\Delta(\tau)$ can be easily found numerically. To find the components of the function \hat{g}_2 one first

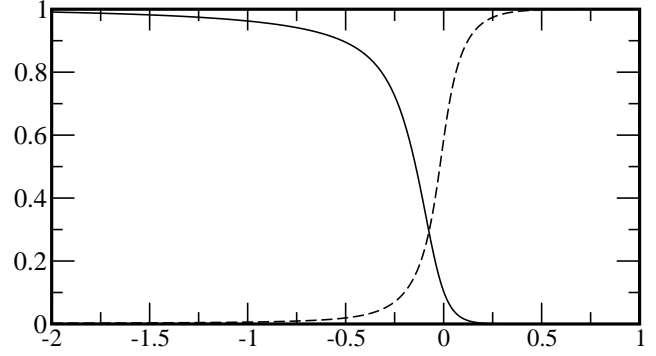


FIG. 2. The normalized order parameter $\Delta(\tau)/\Delta_0$ (dashed line) and the normalized total spin $2S(\tau)/N$ of the grain as functions of on $\tau' = \tau - T$ at the boundary $\tau \sim T$ between the superconducting (left) and paramagnetic (right) states.

needs to solve Eqs.(24) numerically and then find the components \hat{g}_2 according to Eq.(25). Knowing the functions \hat{g}_1 and \hat{g}_2 for a given configuration $\Delta(\tau)$ one can find the self-consistent configuration of $\Delta(\tau)$ satisfying Eq.(16). This self-consistent solution $\Delta(\tau)$ along with the total spin of the grain $S(\tau)$ at the right instanton boundary is presented on Fig.2 (solution at the left boundary can be obtained as the mirror reflection of that on the right one). Substituting the functions $\Delta(\tau)$ and g^I, g^{II} into Eq.(12) and calculating the term $\text{Tr} \ln[\partial_\tau + \mathcal{H}_k]$ by the method described in [8] one obtains the result (1).

Conclusions. In conclusion, we have found the probability of the quantum transition between superconducting and paramagnetic states of a nanometer size superconducting grain weakly coupled to a normal metallic plate. Our result (1) obtained formally in the limit of $T \rightarrow 0$ is general and remain valid at finite temperatures as long as $T \ll \delta E$. At higher temperatures, $\delta E \ll T \ll \Delta$, the characteristic energy δE in the exponent of Eq.(1) has to be substituted by temperature T . However, finding numerical coefficient β in this case requires a more advanced study.

We would like to thank Y. Bazaliy, Ya. M. Blanter, E.M. Chudnovsky, D. Feldman, Y.M. Galperin, A.E. Koshelev, A.I. Larkin, K. Matveev, A. Mel'nikov, V.L. Pokrovsky, and R. Ramazashvili for useful discussions. This work was supported by the U.S. Department of Energy, Office of Science under contract No. W-31-109-ENG-38.

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